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TRANSPORT PROPERTIES IN THE ATMOSPHERE OF JUPITER

Semi-Annual Progress Report

January-June, 1979

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The work accomplished during this reporting period falls into the following categories; (1) testing of the computer program used to obtain transport properties for the Hulburt-Hirschfelder potential, (2) calculation of transport properties for the C_2-C interaction, (3) preliminary calculations for the C_2-C_2 interaction, (4) calculation of transport properties for the C_2H-He interaction, (5) consideration of the effect of inelastic collisions on the transport properties, and (6) the use of the Hulburt-Hirschfelder potential to model ion-atom interactions. The results are discussed in sections I through VI below.

I. USE OF THE HULBURT-HIRSCHFELDER POTENTIAL

It was previously reported[1] that a computer program has been written to calculate transport collision integrals for the accurate Hulburt-Hirschfelder potential. This program has now been tested for a specie for which the transport properties are known over a wide range of temperatures; argon. Using only known spectroscopic constants[2] and the computer program for the Hulburt-Hirschfelder potential, the results for the viscosity, η, shown in the second column of Table 1, are obtained. These can be compared with the experimental results[3] shown in the third column of Table 1.

It is important to emphasize that this good agreement has been obtained without using any adjustable parameters in the potential. The constants σ (the "effective" rigid sphere diameter) and ϵ (the depth of the potential well) are not well defined and better agreement with experiment can be obtained by using these as adjustable parameters. However, the results shown in Table 1 indicate that the computer program for the Hulburt-Hirschfelder potential is reliable.

Results for the C-C interaction, using this potential, are now nearly complete. It was previously reported[1] that this potential will calculate

transport collision integrals for states with a local maximum. Comparisons of the viscosity collision integrals obtained from a best fit of the Morse potential (MP) and for the Hulburt-Hirschfelder (HH) potential are shown in Table 2 for the $^1\Sigma_g^+$ state of C_2 (which does not have a local maximum in the potential) and for the $^1\Sigma_u^-$ state (which does have a local maximum). In both cases the Morse and HH curves give different results but the differences are most drastic for the $^1\Sigma_u^-$ state at "lower" temperatures, indicating that the local maximum (which is not treated by any other empirical potential for which transport properties have been calculated) has a significant effect on the transport properties.

In the previous results for the C-C transport properties,[4] the $^3\Sigma_{u2}^+$ and $^5\Sigma_{g2}^+$ states were ignored since neither experimental nor theoretical information about these states is available. However, the perfect pairing method[5,6,7] makes it possible to obtain information about unknown states from states for which the potential energy curves are known. This method has been used to obtain the potential energy curves for the $^3\Sigma_{u2}^+$ and $^5\Sigma_{g2}^+$ states. The results will be incorporated into the revised results for the C-C transport properties obtained using the computer program for the HH potential.

II. TRANSPORT PROPERTIES FOR THE C_2-C INTERACTION

The transport properties corresponding to the C_2-C interaction have been calculated using the peripheral force model,[8,9] previously discussed.[1,10,11] However, previous results have been improved by using the HH potential to represent all of the C-C states with a potential minimum and the exponential repulsive (ER) potential has been used to represent all the repulsive C-C states.

For the HH potential, the averaged C_2-C interaction potential is given by

$$V(r-HH)_{av} =$$

$$\frac{2\varepsilon}{\alpha(xr)^2} e^{xr_e} [e^{-xr(1+\alpha)}(xr[1+\alpha]+1) - e^{-xr(1-\alpha)}(xr[1-\alpha]+1)]$$

$$+ \frac{\varepsilon}{\alpha} cx^2 e^{2xr_e} [B+E+F+G+H] \tag{1}$$

where

$$B = [(1+\alpha)^5 e^{-2xr(1+\alpha)} - (1-\alpha)^5 e^{-2xr(1-\alpha)}](-\frac{1}{2} bxr^3)$$

$$E = [(1+\alpha)^4 e^{-2xr(1+\alpha)} - (1-\alpha)^4 e^{-2xr(1-\alpha)}]r^2(-\frac{1}{2} - \frac{5b}{4} + 2bxr_e)$$

$$F = [(1+\alpha)^3 e^{-2xr(1+\alpha)} - (1-\alpha)^3 e^{-2xr(1-\alpha)}]r(-\frac{1}{x} + \frac{3}{2} r_e + 4br_e - \frac{5b}{2x} - 3bxr_e^2)$$

$$G = [(1+\alpha)^2 e^{-2xr(1+\alpha)} - (1-\alpha)^2 e^{-2xr(1-\alpha)}]$$

$$\times (-\frac{3}{2x^2} + \frac{9r_e}{4x} - \frac{3r_e^2}{2} + \frac{6br_e}{x} - \frac{9br_e^2}{2} + 2bxr_e^3 - \frac{15b}{4x^2})$$

$$H = [e^{-2xr(1+\alpha)}(2xr[1+\alpha]+1) - e^{-2xr(1-\alpha)}(2xr[1-\alpha]+1)]$$

$$\times (-\frac{1}{4cx^4r^2} - \frac{15b}{8x^4r^2} + \frac{3br_e}{x^3r^2} - \frac{9br_e^2}{4x^2r^2} + \frac{br_e^3}{xr^2} - \frac{3}{4x^4r^2} + \frac{9r_e}{8x^3r^2}$$

$$- \frac{3r_e^2}{4x^2r^2} + \frac{r_e^3}{4xr^2} - \frac{br_e^4}{4r^2})$$

$$x = \frac{\omega_e}{2r_e\sqrt{B_e\varepsilon}} \qquad \alpha = \frac{a}{r} \qquad a_0 = \frac{\omega_e^2}{4B_e}$$

$$a_1 = -1 - \frac{\alpha_e\omega_e}{6B_e^2} \qquad a_2 = \frac{5}{4} a_1^2 - \frac{2\omega_e X_e}{3B_e}$$

$$b = 2 - \frac{\frac{7}{12} - \varepsilon \frac{a_2}{a_0}}{c} \qquad c = 1 + a_1 \sqrt{\frac{\varepsilon}{a_0}}$$

and r_e, ε, B_e, ω_e, $\omega_e X_e$, and α_e are spectroscopic constants. Also, a is half the C-C bond length. For the ER potential, the averaged C_2-C interaction

potential is given by

$$V(r\text{-}ER)_{av} = \frac{A}{aB^2 r} \left[e^{-Br(1-\alpha)} (Br[1-\alpha]+1) - e^{-Br(1+\alpha)}(Br[1+\alpha]+1) \right] \qquad (2)$$

where A and B are the parameters for the ER potential.

Using equations (1) and (2), potential energy curves were obtained for each of the 18 states of C_2. The results obtained using equation (1) were best fit with the Morse potential and the results obtained using equation (2) were best fit with the ER potential. The transport collision integrals for each state were then obtained and averaged according to their degeneracies.[12] The results are given in Table 3.

III. TRANSPORT PROPERTIES FOR THE C_2-C_2 INTERACTION

The peripheral force model can also be applied to the C_2-C_2 interaction. For the states of C_2 that are described by the HH potential, the averaged C_2-C_2 interaction potential is given by

$$V(r\text{-}HH)_{av} = 2\epsilon - \frac{4\epsilon}{\alpha(xr)^2} e^{xr}e[e^{-xr(1+2\alpha)} - e^{-xr}] + \frac{\epsilon cx}{\alpha^2 r} e^{2xr}e[\{(1+2\alpha)^5 e^{-2xr(1+2\alpha)}$$

$$+ (1-2\alpha)^5 e^{-2xr(1-2\alpha)} - 2e^{-2xr}\}(\frac{bxr^3 e}{4}) + \{(1+2\alpha)^4 e^{-2xr(1+2\alpha)}$$

$$+ (1-2\alpha)^4 e^{-2xr(1-2\alpha)} - 2e^{-2xr}\}(\frac{5bx^2}{8} - \frac{1}{2} A) + \{(1+2\alpha)^3 e^{-2xr(1+2\alpha)}$$

$$+ (1-2\alpha)^3 e^{-2xr(1-2\alpha)} - 2e^{-2xr}\}(\frac{5bx}{4r} - \frac{1}{2} B - \frac{A}{xr}) - \{(1+2\alpha)^2 e^{-2xr(1+2\alpha)}$$

$$+ (1-2\alpha)^2 e^{-2xr(1-2\alpha)} - 2e^{-2xr}\}(\frac{1}{2} D + \frac{3B}{4xr} + \frac{3A}{2x^2r^2} + \frac{15b}{8r^2})$$

$$+ \frac{1}{2} E \{(e^{-2xr} - e^{-2xr(1-2\alpha)})(1-2xr\alpha) - (e^{-2xr(1+2\alpha)} - e^{-2xr})(1+2xr\alpha)$$

$$+ e^{-2xr}(2xr[1+\alpha]+1) - e^{-2xr(1-2\alpha)}(2xr[1-\alpha]+1) - e^{-2xr(1+2\alpha)}(2xr[1+\alpha]+1)$$

$$+ e^{-2xr}(2xr[1-\alpha]+1)\} + \{2e^{-2xr}(2xr+1) - e^{-2xr(1+2\alpha)}(2xr[1+2\alpha]+1)$$

$$- e^{-2xr(1-2\alpha)}(2xr[1-2\alpha]+1)\}(\frac{D}{4x^2r^2} + \frac{3A}{2x^2r^2} + \frac{3A}{4x^4r^4} + \frac{15b}{16x^2r^4}) \qquad (3)$$

where

$$A = 2bxr_e r^2 - \frac{5br}{4} - \frac{1}{2}r^2$$

$$B = \frac{5brr_e}{2} - \frac{5br}{2x} + \frac{3rr_e}{2} - \frac{r}{x}$$

$$D = \frac{6br_e}{r} - \frac{15b}{4x^2} - \frac{9br_e^2}{2} + 2bxr_e^2 - \frac{3}{2x^2} + \frac{9r_e}{4x} - \frac{3r_e^2}{2}$$

and

$$E = \frac{9br_e}{2x^2 r} - \frac{15b}{4x^3 r} - \frac{9br_e^2}{4x^2 r^2} - \frac{br_e^3}{2xr^2} - \frac{3}{4x^4 r^3} + \frac{3br_e}{4x^3 r^2} + \frac{9r_e^2}{8x^3 r^2} + \frac{3r_e^2}{4x^2 r^2}$$

$$+ \frac{r_e^2}{4xr^2} - \frac{br_e^4}{4r^2} - \frac{1}{4cx^4 r^2}$$

For the states of C_2 that are described by the ER potential, the averaged C_2-C_2 interaction potential is given by

$$V(r\text{-ER})_{av} = \frac{A}{\alpha^2 B^3 r^3} \left[e^{-Br(1+2\alpha)}(Br[1+2\alpha]+2) + e^{-Br(1-2\alpha)}(Br[1-2\alpha]+2) \right.$$

$$\left. - 2e^{-Br}(Br+2) \right] \tag{4}$$

where

$$\alpha = \frac{a}{r}$$

and A and B are the parameters for the ER potential.

Calculations of the C_2-C_2 transport collision integrals, using equations (3) and (4), are in progress.

IV. TRANSPORT PROPERTIES FOR THE C_2H-He INTERACTION

The C_2H-He interaction has been discussed in some detail previously.[1] The calculations have been refined. These calculations suggest that the contribution of the central (shielded) carbon atom is not large, as discussed previously.[1]

Results have been obtained for three models, using the following labels;

$$C^1 - C^2 - H^3$$
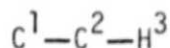
where the superscripts label the atoms.

Model 1

Interactions between He and C^1 and He and H^3 are equally probable and He does not interact with C^2.

Model 2

Interactions of He with C^1, C^2, and H^3 are equally probable.

Model 3

Interactions of He with C^1 and H^3 are equally probable and are twice as probable as interactions of He with C^2.

Using these models, the peripheral force method leads to the results for the transport properties shown in Tables 4, 5, and 6. The results are very similar for all three models.

It is important to attempt to compare these results with other results since the He-C_2H interaction represents a "test case" for use of the peripheral force model for ablation products. Esch, Siripong, and Pike[13] have estimated the collision parameters σ and ϵ for C_2H. They did this by making correlations of σ and ϵ versus molecular weight for species for which these parameters are known. The parameters for helium are given in Hirschfelder, Curtiss, and Bird.[14] Esch, et al.[13] obtained the parameters for the He-C_2H interaction by using the empirical combining laws[14]

$$\sigma_{12} = \frac{1}{2}(\sigma_1 + \sigma_2)$$

and

$$\epsilon_{12} = \sqrt{\epsilon_1 \epsilon_2}$$

They then assumed that the He-C_2H interaction is described by the Lennard-Jones (6,12) potential. Their results for the transport properties are given in Table 7.

The reasonably good agreement between the results in Tables 4-6 and Table 7 may be surprising especially since repulsive interactions (based on experimental data[8,9,15,16]) have been used for the peripheral force calculations while the Lennard-Jones (6,12) potential possesses an attractive minimum. However, it has been shown that the transport properties are relatively insensitive to the nature of the interaction potential.[17,18] Thus the reasonably good agreement obtained using these very different interaction potentials is not entirely unexpected.

Based on the observation that transport properties are relatively insensitive to the details of the interaction potential, Boushehri, Viehland, and Mason[19] have proposed a "universal" set of collision integrals which does not require any assumptions about the functional form of the interaction potential. This set of collision integrals was generated from experimental information about the transport properties of the noble gases but Boushehri, et al.[19] suggest that the transport properties for many polyatomic and polar gases can be accurately estimated using their set of collision integrals. The reason for this is that they found that the relatively featureless repulsive "wall" of the potential (which seems to be more or less the same independent of the nature of the two interacting atoms and/or molecules) determines the viscosity. As a corroboration of the suggestion of Boushehri, et al.[19], a "universal" formula for the viscosity, determined in a similar fashion using noble gas data[20], has been applied to a variety of atom-molecule and molecule-molecule interactions[3,20,21,22,23] with good results.

When the collision integrals given by Boushehri, et al.[19] are applied to the He-C_2H interaction, using the values of σ and ε obtained by Esch, et al.[13] for C_2H and listed in Hirschfelder, et al.[14] for helium, the results shown in Table 8 are obtained. These results agree remarkably well with the results in Tables 4-6. This agreement leads to increased confidence that the peripheral

force model is, indeed, applicable to the He-C_2H interaction although
experimental transport data for this interaction is not available to be used
to verify the results.

The origin of the coordinate system for the He-C_2H interaction has been
taken to be at the geometric center of the molecule. However, Amdur and his
co-workers took the origin to be at the center of mass of the molecule, which
is consistent with the assumption of central forces. But, for the peripheral
force model, the centers of force are located at the individual atoms in the
molecule and there is no particular reason to expect that the orientation
averaged atom-molecule interaction, averaged over all individual atom-atom
interactions, should be "localized" at the center of mass. This is illustrated
by some of the results of Amdur, et al.[15]

Similar to the problems encountered by Amdur, et al.[15], the
attempt to calculate the He-C_2H transport properties by referring the calcu-
lations to the center of mass of C_2H requires the use of physically unreasonable
atom-atom interaction potentials and leads to transport properties that are
considerably different than those predicted using the models of Esch, et al.[13]
and of Boushehri, et al.[19] Amdur, et al.[15] indicate that improvements in the
results may be possible if other representations of the interaction are used,
such as locating the centers of interaction elsewhere in the molecule than at
the nuclei.[24] However, clearly this is essentially a "curve fitting" procedure
and is really no different than locating the origin of the coordinate system
somewhere other than at the center of mass.

Thus there appears to be some arbitrariness in the use of the peripheral
force model, particularly when it is applied to systems for which experimental
information that can be related to interaction potentials is not available.
This arbitrariness is probably primarily due to the fact that each interaction,
involving different chemical species, has unique properties; e.g. the electronic

structure corresponding to each interaction is different. None of the theories of intermolecular interactions available at present is likely to be sensitive to small shifts in electronic structure, at least not without recourse to experimental information. The best way to resolve this arbitrariness in the peripheral force method, for a particular interaction, appears to be to compare results for the transport properties obtained using this method with results obtained using a more "generic" method such as that due to Esch, et al.[13] or Boushehri, et al.[19]

V. INELASTIC EFFECTS ON TRANSPORT PROPERTIES

The effect on the transport properties due to carbon atoms being in different electronic states has been discussed previously.[1,10,11,25] However, the effect of inelastic collisions in which energy is transferred between the translational and electronic degrees of freedom was never explicitly considered; i.e., only the first order approximation for the transport properties,[26] for quasi-elastic collisions, was considered.

In the second order approximation[26]

$$\lambda_{tr} \left(1 - \frac{Y^2}{XZ}\right) = \frac{75k^2T}{8mX} + \frac{15k c_{int} Y}{4mXZ} \tag{5}$$

and

$$\lambda_{int} \left(1 - \frac{Y^2}{XZ}\right) = \frac{3c_{int}^2 T}{2mZ} + \frac{15kT c_{int} Y}{4mXZ} \tag{6}$$

where

$$X = \frac{5kT}{2\eta} + \frac{25c_{int}}{12nk\tau} \tag{7}$$

$$Y = \frac{5c_{int}}{4nk\tau} \tag{8}$$

and

$$Z = \frac{3c_{int} T}{2\rho D} + \frac{3c_{int}}{4nk\tau} \tag{9}$$

Also, τ is the relaxation time (electronic-translational relaxation in this case) which depends explicitly on the inelastic collision process. In addition the collision number, Z_{elec} (which roughly gives the number of collisions required to interchange a quantum of electronic energy with translational energy), is given by[26]

$$Z_{elec} = \frac{4p\tau}{\pi\eta} \qquad (10)$$

Since Z_{elec} involves the ratio τ/η, systematic errors made in evaluating τ and η should tend to cancel. Using a rigid sphere model for evaluating τ and η, it is found that

$$Z_{elec} = \frac{32\ c_{int}}{5\pi k} \left(\frac{kT}{\Delta E_{elec}}\right)^2 \qquad (11)$$

where ΔE_{elec} is the energy separation of two electronic energy levels.

When these results are used together with the appropriate parameters for the ground and first excited electronic states of carbon, the results shown in the second and third columns of Table 9 are obtained. These results are compared with the rigid sphere results in the first order approximation[25] (columns four and five in Table 9).

Clearly the results are different. Thus it would be useful to be able to evaluate equation (10) for models that are more realistic than the rigid sphere model. An investigation of this problem is currently in progress.

VI. ATOM-ION POTENTIALS

The ability of the Hulburt-Hirschfelder curve to accurately reproduce experimental potential energy curves for atom-atom interactions[7,27] suggests that this potential might accurately reproduce experimental atom-ion potentials. Results for some simple atom-ion interactions are given below.

The spectroscopic constants for the H-H$^+$ interaction are available.[2] These constants give the HH potential shown in Table 10 which are compared with the exact results.[28] The comparison is quite good.

The spectroscopic constants for the He-H$^+$ interaction are available.[2] These constants give the HH potential shown in Table 11 which are compared with the theoretical results.[29] The comparison is quite good.

The spectroscopic constants for the He-He$^+$ interaction are available. These constants give the HH potential shown in Table 12 which are compared with the theoretical results.[30,31] The comparison is quite good.

These results, for small systems, suggest that the Hulburt-Hirschfelder curve may be useful for representing ion-atom interactions. Thus this potential should be tested for bigger systems. In general, potential energy curves for interactions involving "big" atoms and ions are not known. However experimental transport (particularly mobility) data is often available. This is the case for the Hg$^+$-Ar interaction.[32,33] The spectroscopic constants are available for this interaction.[2] These constants give the HH potential shown in Table 13. The HH potential will be used to calculate the transport properties for this system which will be compared with the experimental results, providing a good test of the accuracy of the Hulburt-Hirschfelder potential for atom-ion interactions.

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Table 1

Viscosity, η, of Argon for the Hulburt-Hirschfelder Potential

η(millipoise)

T(°K)	η(Hulburt-Hirschfelder)	η(experimental)*
298.2	244.1	226.1
373.2	291.0	273.2
473.2	347.2	329.2
573.2	398.3	378.9
673.2	445.1	425.1
773.2	489.1	467.6
873.2	530.7	505.8
973.2	570.3	544.0

*These results are from Kestin, et al.[3]

Table 2

Viscosity Collision Integrals, $\sigma^2\Omega^{(2,2)*}$ for the $^1\Sigma_g^+$ and $^1\Sigma_u^-$ States

of C_2 for the Morse and Hulburt-Hirschfelder Potentials

T(°K)	$^1\Sigma_g^+$		$^1\Sigma_u^-$	
	$\sigma^2\Omega^{(2,2)*}$(MP)	$\sigma^2\Omega^{(2,2)*}$(HH)	$\sigma^2\Omega^{(2,2)*}$(MP)	$\sigma^2\Omega^{(2,2)*}$(HH)
1,000	11.5269	7.8147	15.1424	6.9240
5,000	7.7398	4.4743	10.1799	5.4879
10,000	6.4829	4.0782	7.6073	5.0639
15,000	5.6879	3.8505	5.9453	4.5940
20,000	5.0234	3.5030	4.8883	4.1608
25,000	4.4090	3.2033	4.2205	3.8041

The collision integrals are in $\overset{\circ}{A}{}^2$.

Table 3

Transport Collision Integrals for the C_2-C_2 Interaction

$T(10^{-3}{}^{\circ}K)$	$\sigma^2\Omega(1,1)^*(\mathring{A}^2)$	$\sigma^2\Omega(2,2)^*(\mathring{A}^2)$	A^*	B^*
1	10.9159	12.3063	1.1310	1.1197
2	9.5378	10.6120	1.1232	1.1357
3	8.7476	9.7077	1.1202	1.1468
4	8.1928	9.0751	1.1194	1.1579
5	7.7548	8.5858	1.1203	1.1708
6	7.3954	8.1976	1.1223	1.1834
7	7.1098	7.8987	1.1255	1.1972
8	6.8408	7.6229	1.1295	1.2093
9	6.6018	7.3817	1.1333	1.2187
10	6.3899	7.1739	1.1376	1.2297
11	6.1933	6.9806	1.1417	1.2370
12	6.0584	6.8512	1.1451	1.2476
13	5.8777	6.6728	1.1489	1.2516
14	5.7045	6.5007	1.1527	1.2548
15	5.5504	6.3467	1.1554	1.2571
16	5.4062	6.2019	1.1584	1.2586
17	5.2741	6.0681	1.1609	1.2594
18	5.1490	5.9403	1.1634	1.2606
19	5.0335	5.8212	1.1655	1.2605
20	4.9233	5.7072	1.1675	1.2604
21	4.8246	5.6064	1.1696	1.2616
22	4.7178	5.4938	1.1716	1.2606
23	4.6257	5.3959	1.1731	1.2595
24	4.5280	5.2918	1.1744	1.2535
25	4.4400	5.1968	1.1758	1.2569

Table 4

Transport Properties for the He-C_2H Interaction

Model 1

T(10^{-3}°K)	D($10^2 m^2$/sec)*	η(10^4kg/m/sec)	λ_{tr}(W/m/°K)
1	0.051	0.3114	0.1407
2	0.165	0.5011	0.2264
3	0.328	0.6620	0.2990
4	0.533	0.8065	0.3643
5	0.776	0.9400	0.4246
6	1.055	1.065	0.4813
7	1.369	1.184	0.5350
8	1.714	1.298	0.5863
9	2.091	1.407	0.6357
10	2.498	1.513	0.6834
11	2.933	1.615	0.7296
12	3.397	1.715	0.7745
13	3.888	1.811	0.8183
14	4.405	1.906	0.8610
15	4.949	1.998	0.9027
16	5.518	2.089	0.9436
17	6.112	2.178	0.9837
18	6.731	2.265	1.0231
19	7.373	2.350	1.0618
20	8.039	2.435	1.0999
21	8.729	2.518	1.1373
22	9.441	2.599	1.1742
23	10.177	2.680	1.2106
24	10.934	2.759	1.2465
25	11.713	2.838	1.2819

*D is calculated for 1 atmosphere pressure.

Table 5

Transport Properties for the He-C_2H Interaction

Model 2

$T(10^{-3}°K)$	$D(10^2 m^2/sec)$*	$\eta(10^4/kg/m/sec)$	$\lambda_{tr}(W/m/°K)$
1	0.049	0.2974	0.1343
2	0.159	0.4814	0.2175
3	0.317	0.6382	0.2883
4	0.517	0.7795	0.3521
5	0.754	0.9103	0.4112
6	1.026	1.0333	0.4668
7	1.333	1.1501	0.5196
8	1.671	1.2620	0.5701
9	2.041	1.3697	0.6187
10	2.441	1.4738	0.6658
11	2.868	1.5747	0.7114
12	3.324	1.6729	0.7557
13	3.807	1.7686	0.7990
14	4.316	1.8621	0.8412
15	4.852	1.9536	0.8825
16	5.413	2.0433	0.9230
17	5.999	2.1312	0.9627
18	6.610	2.2176	1.0018
19	7.244	2.3025	1.0401
20	7.902	2.3862	1.0779
21	8.584	2.4684	1.1151
22	9.288	2.5496	1.1517
23	10.015	2.6296	1.1879
24	10.764	2.7085	1.2235
25	11.535	2.7865	1.2588

*D is calculated for 1 atmosphere pressure.

Table 6

Transport Properties for the He-C_2H Interaction

Model 3

$T(10^{-3}°K)$	$D(10^2 m^2/sec)*$	$\eta(10^4 kg/m/sec)$	$\lambda_{tr}(W/m/°K)$
1	0.050	0.3043	0.1375
2	0.162	0.4912	0.2219
3	0.323	0.6501	0.2937
4	0.525	0.7931	0.3582
5	0.765	0.9253	0.4180
6	1.041	1.0495	0.4741
7	1.351	1.1675	0.5274
8	1.693	1.2803	0.5784
9	2.066	1.3889	0.6274
10	2.470	1.4938	0.6748
11	2.901	1.5955	0.7207
12	3.361	1.6943	0.7654
13	3.849	1.7907	0.8089
14	4.362	1.8848	0.8514
15	4.902	1.9768	0.8930
16	5.467	2.0670	0.9337
17	6.057	2.1554	0.9737
18	6.673	2.2422	1.0129
19	7.311	2.3275	1.0514
20	7.973	2.4115	1.0894
21	8.659	2.4942	1.1267
22	9.368	2.5757	1.1635
23	10.100	2.6560	1.1998
24	10.853	2.7353	1.2356
25	11.629	2.8136	1.2710

*D is calculated for 1 atmosphere pressure.

Table 7

Transport Properties for the He-C_2H Interaction

Lennard-Jones(6,12) Potential*

$T(10^{-3}$°K)	$D(10^2 m^2$/sec$)^{**}$	$\eta(10^4$kg/m/sec)	λ_{tr}(W/m/°K)
1	0.046	0.290	0.131
2	0.146	0.454	0.205
3	0.286	0.590	0.266
4	0.460	0.710	0.321
5	0.666	0.820	0.370
6	0.900	0.922	0.416
7	1.16	1.02	0.460
8	1.45	1.11	0.501
9	1.76	1.20	0.541
10	2.10	1.28	0.579
11	2.45	1.36	0.616
12	2.83	1.44	0.651
13	3.24	1.52	0.686
14	3.66	1.59	0.719
15	4.10	1.66	0.752
16	4.56	1.74	0.784
17	5.05	1.80	0.815
18	5.55	1.87	0.846
19	6.07	1.94	0.876
20	6.60	2.00	0.905
21	7.16	2.07	0.934
22	7.73	2.13	0.963
23	8.32	2.19	0.991
24	8.93	2.25	1.02
25	9.55	2.31	1.05

*These results were obtained using the parameters for C_2H suggested by Esch, et al.[13] and the parameters for He given in Hirschfelder, et al.[14]

**D is calculated for 1 atmosphere pressure.

Table 8

Transport Properties for the He-C_2H Interaction

"Universal" Collision Integrals*

$T(10^{-3}{}^\circ K)$	$D(10^2 m^2/sec)$**	$\eta(10^4 kg/m/sec)$	$\lambda_{tr}(W/m/{}^\circ K)$
1	0.048	0.292	0.132
2	0.154	0.468	0.210
3	0.307	0.622	0.278

*The transport collision integrals used are those given by Boushehri, et al.[19], the C_2H parameters used are those given by Esch, et al.[13], and the He parameters used are those given by Hirschfelder, et al.[14]

**D is calculated for 1 atmosphere pressure.

Table 9

Thermal Conductivity of Monatomic Carbon at 1 Atmosphere Pressure

$$\lambda(W/m/^{\circ}K)$$

$T(10^{-3}{}^{\circ}K)$	$\lambda_{tr}(in)$	$\lambda_{int}(in)$	$\lambda_{tr}(rs)$	$\lambda_{int}(rs)$
5	0.126	0.022	0.145	0.012
10	0.176	0.042	0.205	0.028
15	0.214	0.145	0.251	0.127
20	0.259	0.344	0.290	0.327
25	0.301	0.442	0.325	0.421

Table 10

The H-H$^+$ Interaction Potential

r(a.u.)	V(HH-hartrees)	V(exact-hartrees)*
0.05	2.366	2.259
0.50	0.597	0.576
1.00	0.050	0.044
1.50	-0.078	-0.083
2.00	-0.097	-0.103
2.50	-0.088	-0.094
3.00	-0.072	-0.077
3.80	-0.046	-0.051
4.60	-0.027	-0.030
6.20	-0.008	-0.010
7.00	-0.004	-0.005

*The exact results are from Wind.[28]

Table 11

The He-H$^+$ Interaction Potential

r(a.u.)	V(HH-hartrees)	V(theory-hartrees)*
0.10	6.218	15.770
0.50	0.874	0.968
1.00	0.005	0.004
1.25	-0.058	-0.059
1.75	-0.059	-0.059
2.00	-0.046	-0.045
3.00	-0.011	-0.012
4.00	-0.002	-0.004
6.00	0	-0.001

*The theoretical results are from Michels.[29]

Table 12

The He-He$^+$ Interaction Potential

r(a.u.)	V(HH-hartrees)	V(theory-hartrees)*
0.50	2.095	2.377
1.00	0.348	0.351
1.40	0.009	
1.50		-0.023
1.75		-0.071
1.80	-0.079	
2.20	-0.085	
2.25		-0.082
2.50	-0.073	-0.072
3.00	-0.049	-0.049
4.00	-0.017	-0.018
5.00	-0.006	-0.005

*The theoretical results are from Gupta and Matsen.[30,31]

Table 13

The (HgAr)$^+$ Interaction Potential

r(a.u.)	V(HH-hartrees)
4.1	0.0079
4.2	0.0074
4.3	0.0059
4.5	0.0017
5.0	-0.0059
5.5	-0.0073
6.0	-0.0061
6.5	-0.0043
7.0	-0.0029
7.5	-0.0019
8.0	-0.0013
9.0	-0.0005
10.0	-0.0002